

Chapter 10

Process-Based Modeling of Nutrient Cycles and Food-Web Dynamics

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Abstract Mathematical models are indispensable for addressing pressing aquatic ecosystem management issues, such as understanding the oceanic response to climate change, the interplay between plankton dynamics and atmospheric CO₂ levels, and alternative management plans for eutrophication control. The appeal of process-based (mechanistic) models mainly stems from their ability to synthesize among different types of information reflecting our best understanding of the ecosystem functioning, to identify the key individual relationships and feedback loops from a complex array of intertwined ecological processes, and to probe ecosystem behavior using a range of model application domains. Significant progress in developing and applying mechanistic aquatic biogeochemical models has been made during the last three decades. Many of these ecological models have been coupled with hydrodynamic models and include detailed biogeochemical/biological processes that enable comprehensive assessment of system behavior under various conditions. In this chapter, case studies illustrate ecological models with different spatial configurations. Given that each segmentation depicts different trade-offs among model complexity, information gained, and predictive uncertainty, our objective is to draw parallels and ultimately identify the strengths and weaknesses of each strategy.

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10.1 Introduction

Mechanistic aquatic biogeochemical models have formed the scientific basis for environmental management decisions by providing a predictive link between management actions and ecosystem responses. An appealing feature for their extensive use is their role as “information integrators” in that they can be used to synthesize across different types of information that reflect our best understanding of ecosystem functioning (Spear 1997). Their main foundation consists of causal mechanisms, complex interrelationships, and direct and indirect ecological paths that are mathematically depicted in the form of nonlinear differential equations. Model endpoints (*state variables*) usually coincide with routinely monitored environmental variables that, in turn, are considered reliable surrogates of the physics, chemistry and biology of the aquatic ecosystem under investigation. Scientific knowledge, expert judgment, and experimental/field data are used to assign realistic values to model inputs. Such inputs can either be ecologically meaningful *parameters*, representing physical or chemical processes, physiological rates, and partition coefficients, or factors that externally influence the biotic and abiotic components of the system, also known as *forcing functions*. The latter model input could be essential in linking an externally-introduced pollutant (e.g., herbicide application or nutrient loading rates) with a key ecosystem attribute (e.g., biodiversity, total phytoplankton or cyanobacteria levels) or may not be directly subject to anthropogenic control, e.g., temperature and solar radiation.

In the context of environmental decision-making and management, the state variables of a model typically represent components or attributes of the system that we consider to be relevant to the research question being examined. For example, in lake eutrophication problems, the state variables can be the various forms of phosphorus (phosphate, dissolved and particulate organic phosphorus) and the different phytoplankton (diatoms, green algae, cyanobacteria) or zooplankton (copepods, cladocerans) groups. If we are interested in predicting the success of a strategy to reduce fish contamination levels in the Great Lakes, then logical state variables of the model will be the contaminant concentrations in the tissues of several fish species along with their corresponding biomass levels. The state variables can be expressed in units of mass or concentration (*biogeochemical models*), energy (*bioenergetic models*), and number of species or individuals per unit of volume or area (*biodemographic models*). Consequently, the physical, chemical, and biological processes considered by the model account for the transfer of mass, energy and/or individuals and drive the variability of the state variables. Examples of physical processes are diffusive and advective transport of a fluid such as air or water; chemical reactions typically modeled are hydrolysis, photolysis, oxidation, and reduction; biological processes that are essential in modulating the dynamics of biotic components are growth, metabolism, mortality, excretion, predation, and emigration or immigration.

An interesting feature of mathematical models is the existence of *feedback loops* (defined as closed-loop circles of cause and effect in ecological conditions in one

part of the system that shape processes elsewhere in the system) that amplify (*positive feedbacks*) or counteract (*negative feedbacks*) the original change. A characteristic example is the positive feedback of bacteria-mediated mineralization of the excreta of zooplankton basal metabolism that replenishes the summer epilimnetic phosphate pool, which stimulates phytoplankton growth and offsets the herbivorous control of autotroph biomass. Then, this increase of the phytoplankton biomass reinforces the zooplankton growth, thereby preventing an undesirable collapse at the second trophic level. An example of a negative feedback in the system is when excessive phosphorus is added causing excessive phytoplankton growth which, in turn, causes shading that reduces sunlight penetration to lower water depths and therefore the reduced primary production along with the decomposition of the sinking phytoplankton cells result in gradual oxygen depletion and possibly hypolimnetic anoxia which could kill off benthic organisms. Thus, the ability of mathematical models to consider a series of intermingled ecological mechanisms allows reproducing non-linear response patterns induced by distant (and presumably unrelated) causal factors.

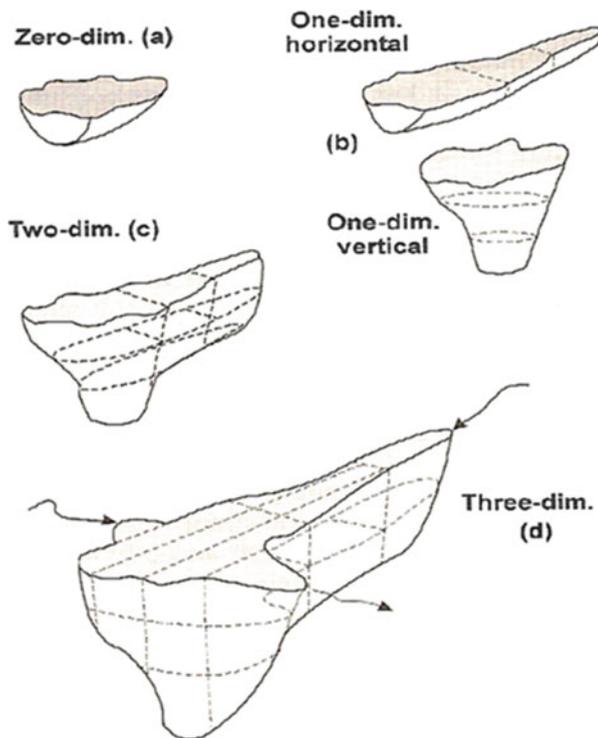
Fundamental to mathematical models is the *Lomonosov-Lavoisier Law of Conservation of Mass*. In quantitative terms, the principle is translated into a *mass balance model* that is built from *mass balance equations* that account for all the inputs and outputs of mass across the system's boundaries and all the transport and transformation processes occurring within the system. For a finite period of time, this concept can be mathematically expressed as:

$$\begin{aligned} \text{Accumulation} &= \Delta \text{Mass} / \Delta t = \Delta(\text{Volume} \cdot \text{Concentration}) / \Delta t \\ &= \text{Input} \pm \text{Reactions} - \text{Output} \end{aligned}$$

This differential equation is solved to get model output (concentration) as a function of time. The solution provides us with a *time dependent, dynamic or unsteady-state model* (these terms are used interchangeably). If the equation is relatively simple, then we can mathematically solve the equation to get an *explicit analytical solution* where infinitesimal time steps are implied. However, often the equation(s) are difficult to solve, in which case we use *numerical approximations*. The simplest of these numerical methods is a *finite difference* approach whereby the computer algorithm steps through time according to defined and discrete time steps. An alternative solution to explicitly solving a differential equation is to assume no change in the state variable value with time or that the system is at a *steady state*, i.e., $\Delta \text{Mass} / \Delta t = 0$.

Mathematical models must also consider variations in space (e.g., geographic variation). If we do not consider spatial variation, then we have a *lumped model*, e.g., $\Delta \text{Mass} / \Delta x = 0$ where x is distance. An example of a lumped model would be treating a lake's water column as a single well-mixed compartment, i.e., the contents are sufficiently well mixed as to be uniformly distributed (Fig. 10.1a). Such characterization is often used to model shallow and small lakes, where stratification does not occur and spatial homogeneity can be assumed. A common example of this type of models is the *continuously stirred tank reactor* (CSTR) that

Fig. 10.1 Zero-, one-, two-, and three-dimensional strategies for accommodating the spatial variability in lake systems



simulates the system as a single, well-mixed or homogeneous compartment, where its properties can only vary in time according to the following equation:

$$\frac{dC}{dt} = f(C, \theta, t)$$

where the quantity C (e.g. chemical concentration) being differentiated is called the *dependent variable*; the quantity t (time in zero-dimensional systems) with respect to which C is differentiated is called the *independent variable*, and θ corresponds to the various inputs of the equation (e.g. external forcing, parameters). When the function involves one independent variable the equation is called *ordinary differential equation* (or ODE). Alternatively, we may consider spatial variations, with the simplest formulation of translating geographic differences into discrete, well-mixed (homogeneous) boxes or compartments, typically defined according to physical properties of the studied system. This type of model is often called a *box model*. Using a lake as an example, a box model may have a warmer upper water layer or epilimnion and a cooler lower water layer or hypolimnion to treat thermal stratification (Fig. 10.1c). In this example, the *discretisation* is defined according to the temperature vertical profiles. The model

then includes heat and/or chemical transfer between the two compartments according to heat and mass transfer coefficients.

The most sophisticated treatment of spatial variation is to have an analytical solution to the differential $dMass/dx$. This would quantify the continuous variation in the output as a function of space or location and hence would offer a *continuous model*. Similarly to solutions of the time-varying differential equation, we can solve the equations using an explicit analytical solution or a numerical approximation. In this case, we deal with *partial differential equations* (or PDE) that involve two or more independent variables. For example, such equations can be useful for systems with a prevailing one-directional flow, e.g., rivers where the physical, chemical, and biological properties are determined by this flow, and thus we may opt for a one-dimensional representation that accommodates variability in the x axis (Fig. 10.1b). Namely, the advection-diffusion equation that combines the two main processes of mass transport, advection and diffusion, along with a first-order reaction, will be suitable to describe the spatiotemporal distribution of a substance in a river:

$$\frac{\partial C}{\partial t} = -\frac{\partial Cu}{\partial x} + D_x \frac{\partial^2 C}{\partial x^2} - kC$$

where C the chemical concentration in fixed element of space, x (distance) the direction of the flow, u (distance/time) is velocity for advective transport, D_x (distance²/time) is a diffusion coefficient for diffusive transport, and k (inverse time) is a rate constant for a first-order reaction. One-dimensional representations can also be used to simulate the vertical stratification of a deep lake without significant variability in the horizontal plane (Fig. 10.1b). Two or three-dimensional segmentations will be more appropriate for larger systems (estuaries, large lakes with complex morphology, fragmented landscapes) characterized by significant variability of their properties in both horizontal and vertical directions (Fig. 10.1c, d). In this chapter, we offer a series of case studies that illustrate ecological models with different spatial configurations. Given that each segmentation depicts different trade-offs among model complexity, information gained, and predictive uncertainty, our objective is to draw parallels and ultimately pinpoint the strengths and weaknesses of each strategy.

10.2 Zero- and One-Dimensional Lake Models

10.2.1 Zero-Dimensional Model for the Phosphorus Cycle in a Hypereutrophic Wetland

Cootes Paradise is a large marsh in western Lake Ontario that is hydraulically connected to Hamilton Harbour by a man-made channel (Fig. 10.2). It is characterized by hypereutrophic conditions, stemming from the agricultural and urban

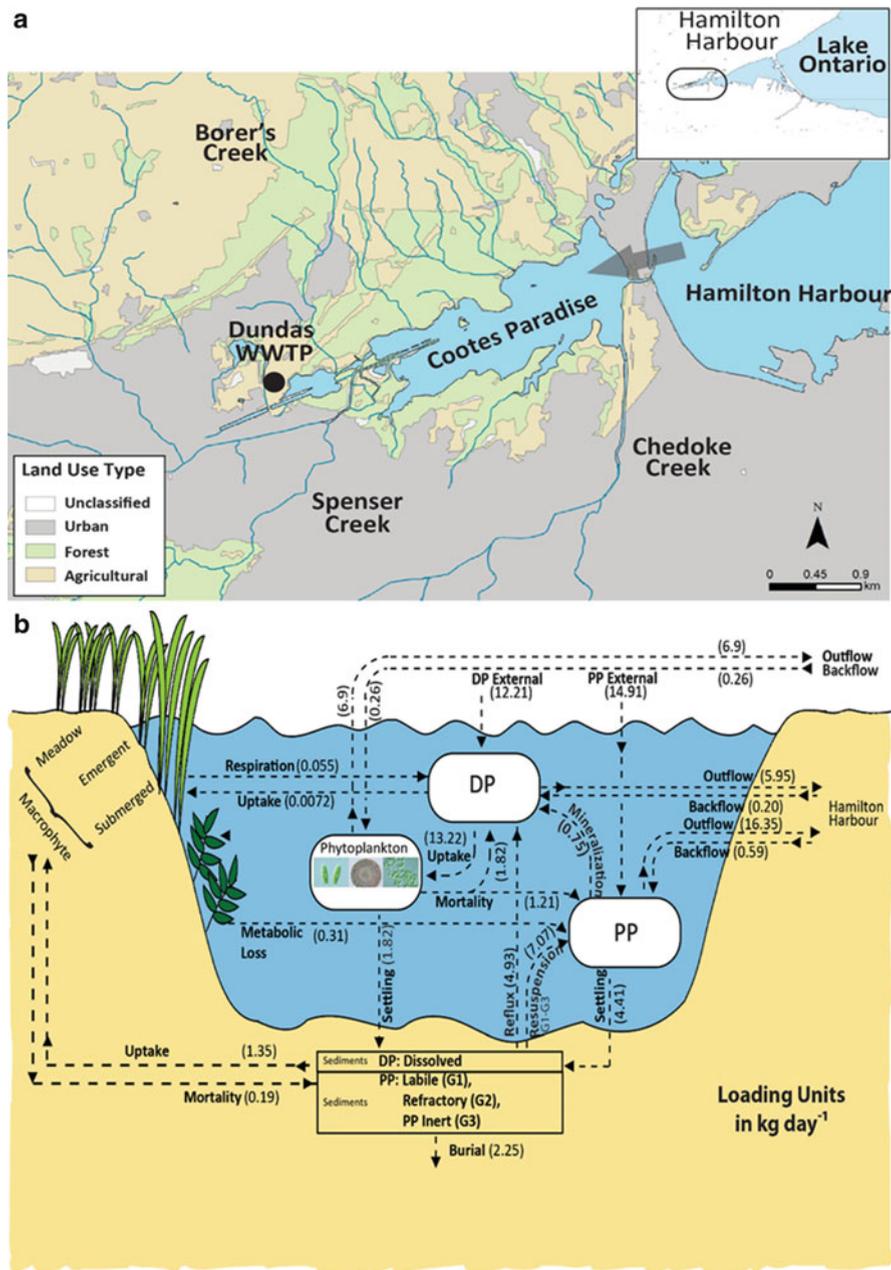


Fig. 10.2 Map of Cootes Paradise and land use classification of the surrounding watershed (a). Average daily phosphorus fluxes (kg day⁻¹) corresponding to each simulated process during the growing season (May–October) (b)

development of the (previously forested) watershed along with the sewage effluent discharged into the marsh for over nine decades (Thomasen and Chow-Fraser 2012). The vegetation cover in Cootes Paradise had receded to less than 15% by the 1990s, relative to >90% cover with very high plant diversity at the turn of the twentieth century (Chow-Fraser 2005). Coinciding with the vegetation decline, the fishery shifted from a desirable warm water fishery of northern pike and largemouth bass to one dominated by planktivorous and benthivorous species, such as bullheads, invasive common carp, and alewife. In particular, common carp, an exotic species introduced into Lake Ontario at the end of the nineteenth century, accounted for up to 45% of the overall water turbidity (Lougheed et al. 2004). High turbidity had many detrimental effects across the entire food web, such as reducing light penetration to a level that was insufficient for submersed aquatic vegetation/periphyton growth, clogging filter-feeding structures of invertebrates, and affecting the behaviour and survival of visually hunting predators and mating fish (Thomasen and Chow-Fraser 2012). To ameliorate the prevailing adverse ecological conditions in the wetland, a number of restoration strategies have been implemented, such as carp exclusion, nutrient loading reduction, and macrophyte planting (Lougheed et al. 2004).

In this context, Kim et al. (2016) presented a modelling exercise aimed at understanding the primary drivers of eutrophication in Cootes Paradise by elucidating the interplay between various phosphorus-loading sources, internal flux rates, phytoplankton activity, and the potential of macrophytes to become an integral part of the bottom-up forcing into the system. Cootes Paradise marsh is approximately 4 km long, with a maximum width of 1 km, and a mean depth of 0.7 m. Because of its small size, the surface area and volume of the marsh can vary significantly according to water level fluctuations, reaching a maximum of 2.5 km² and 3.6 × 10⁶ m³, respectively (Mayer et al. 2005). Thus, Kim et al. (2016) adopted a zero-dimensional approach representing the Cootes Paradise as a spatially homogeneous system with a hydraulic connection to Hamilton Harbour. The focal points of the model calibration were the reproduction of the water level variability and the realistic characterization of processes such as phosphorus release via reflux/diffusion and resuspension from the sediments. The role of macrophytes in the phosphorus cycle was accounted for by the dry-mass biomass submodel presented by Asaeda et al. (2000), and modified by Kim et al. (2013), by differentiating among three macrophyte functional groups: emergent, meadow, and submerged. Each equation considers macrophyte growth through uptake of dissolved inorganic phosphorus from the interstitial water, respiration releasing phosphorus back to the water column, and mortality depositing phosphorus to the sediment pool.

After the model calibration against a 17-year (1996–2012) time-series of water quality data, the Cootes Paradise model provided internal loading estimates ($\approx 12.01 \text{ kg day}^{-1}$) that were substantially lower than sediment reflux rates reported in previous modelling work from the 1990s (Prescott and Tsanis 1997). This discrepancy was attributed to the sediment resuspension induced by carp bioturbation, which ceased after the construction of a barrier (or fishway) at the outlet of Cootes Paradise. The fishway became operational during the winter of 1997 and

used 5-cm wide grating to physically exclude large fish, targeting carp, from the marsh (Lougheed et al. 2004). This biomanipulation practice effectively prevented large carp (>40 cm) from entering the marsh after February 1997. According to the Cootes Paradise marsh model projections (Fig. 10.2), the phosphorus contribution of internal sources (reflux, resuspension, macrophyte respiration) and sinks (sedimentation) appears to be significantly lower relative to the external sources (exogenous inflows) and sinks (outflows to Hamilton Harbour). Release of phosphorus from actively growing submerged and emergent macrophytes is typically considered minimal, whereas decaying macrophytes may act as an internal phosphorus source adding considerable quantities of phosphorus into the water (Granéli and Solander 1988; Asaeda et al. 2000). Nonetheless, the Cootes Paradise model demonstrated that macrophytes play a minimal role in the phosphorus budget of the marsh, reflecting the fact that their abundance (e.g., biomass and density) is fairly low in its current state.

Kim et al. (2016) identified the water level fluctuations as another critical factor that can profoundly modulate the interplay among physical, chemical, and biological components of the Cootes Paradise ecosystem. Lower water levels (and thus smaller water volumes) imply lower dilution and higher nutrient concentrations; a pattern consistent with Kim et al.'s (2016) predictions of higher ambient *TP* values towards the end of the summer-early fall, when the lower water levels in the marsh occur. Further, with lower water levels, wind energy is more easily transmitted to the bottom sediments that, in turn, would accentuate the release of phosphorus due to stirring and mixing (Prescott and Tسانيس 1997; Chow-Fraser 2005). The same mechanisms also appear to be the main drivers of the spatiotemporal variability of water turbidity, thereby influencing the illumination of the water column; especially, the light environment near the sediment surface in open-water sites, which currently does not favour submerged macrophyte growth (Chow-Fraser 2005). In the same context, two threshold water levels have been proposed for evaluating the resilience of submerged macrophytes; a maximum threshold, above which light availability becomes limiting, and a minimum threshold, below which conditions are excessively dry (Harwell and Havens 2003). On a final note, the simplified segmentation of the Cootes Paradise model did not allow researchers to reproduce the water quality gradients occasionally established between western and eastern ends of the marsh. This weakness was highlighted by Kim et al. (2016) as a key missing point that may not allow delineation of the role of a wastewater treatment plant located in the innermost section of Cootes Paradise.

10.2.2 One-Dimensional Model for Nutrient Cycles and Plankton Dynamics in Lakes and Reservoirs

The model SALMO (Benndorf and Recknagel 1982; Recknagel and Benndorf 1982) is a process-based one-dimensional lake model that simulates concentrations of the state variables $\text{PO}_4\text{-P}$, $\text{NO}_3\text{-N}$, DO, detritus, chlorophyta, bacillariophyta,

cyanophyta and cladocera (Fig. 10.3) at daily time steps for the mixed total water body, and epi- and hypolimnion during thermal stratification (Fig. 10.4).

The mass balances for the nutrients and detritus are determined by transport processes such as import, export, sedimentation and exchange between epi- and hypolimnion, as well as consumption by phytoplankton, microbial recycling of detritus and resuspension from anaerobic sediments.

Detritus is also subject to grazing by zooplankton. The mass balances for the phytoplankton phyla chlorophyta, bacillariophyta and cyanophyta, and for cladocera include transport processes by sedimentation, import and export, but are predominantly determined by photosynthesis, respiration and grazing, as well as assimilation, respiration and mortality, respectively. The zooplankton mortality includes predation by planktivorous fish represented by parameters reflecting an annually constant stock size. The DO budget is determined by O₂ solubility (Henry's Law), plankton photosynthesis, and respiration. SALMO requires daily input data for volumes, mean and maximum depths of mixed and stratified water bodies, loadings of PO₄-P, NO₃-N, and detritus by the inflowing water, incident solar radiation and water temperature.

Model inputs (see Fig. 10.3) characterise lake specific nutrient loadings, climate conditions, seasonal circulation types, and morphometry by routinely measured variables. Model parameters reflect lake specific underwater light transmission, temperature, light and nutrient limitations of phyla-specific phytoplankton growth, temperature and food limitation of cladocera growth, stock size of planktivorous fish, specific sinking velocities and grazing preferences for phytoplankton phyla and detritus. The model can therefore easily be implemented and validated for different lakes and drinking water reservoirs based on routine limnological measurements, and can serve as a flexible tool for scenario analysis of eutrophication management options such as control of external and internal nutrient loadings (e.g. Recknagel et al. 1995; Chen et al. 2014) and climate change, artificial destratification and aeration, food web manipulation by carnivorous fish, hypolimnetic withdrawal and partial drawdown (see Chap. 16).

Figures 10.5 and 10.6 display examples for applications of SALMO to a variety of lakes and reservoirs with different circulation types and trophic states. The Saldenbach Reservoir (Germany) had been a key water body during the development and testing phase of SALMO (e.g. Recknagel and Benndorf 1982). As illustrated in Fig. 10.5, the one-dimensional mode of SALMO simulated concentrations of PO₄-P, phyto- and zooplankton separately for epi- and hypolimnion for summer months while the zero-dimensional mode simulated the remaining months of the year 1975. In the case of Lake Taihu (China), the zero-dimensional mode of SALMO simulated successfully extreme conditions of that shallow hypertrophic water body as prerequisite for a scenario analysis on management options (Chen et al. 2014). Again different conditions had to be matched by SALMO when applied to the two warm-monomictic Millbrook and Mt Bold Reservoirs in Australia (Fig. 10.6). The Millbrook Reservoir is equipped with an aerator that artificially destratifies the water body during summer being simulated by the zero-dimensional SALMO. The Millbrook Reservoir will be revisited in Chap. 16 when the model

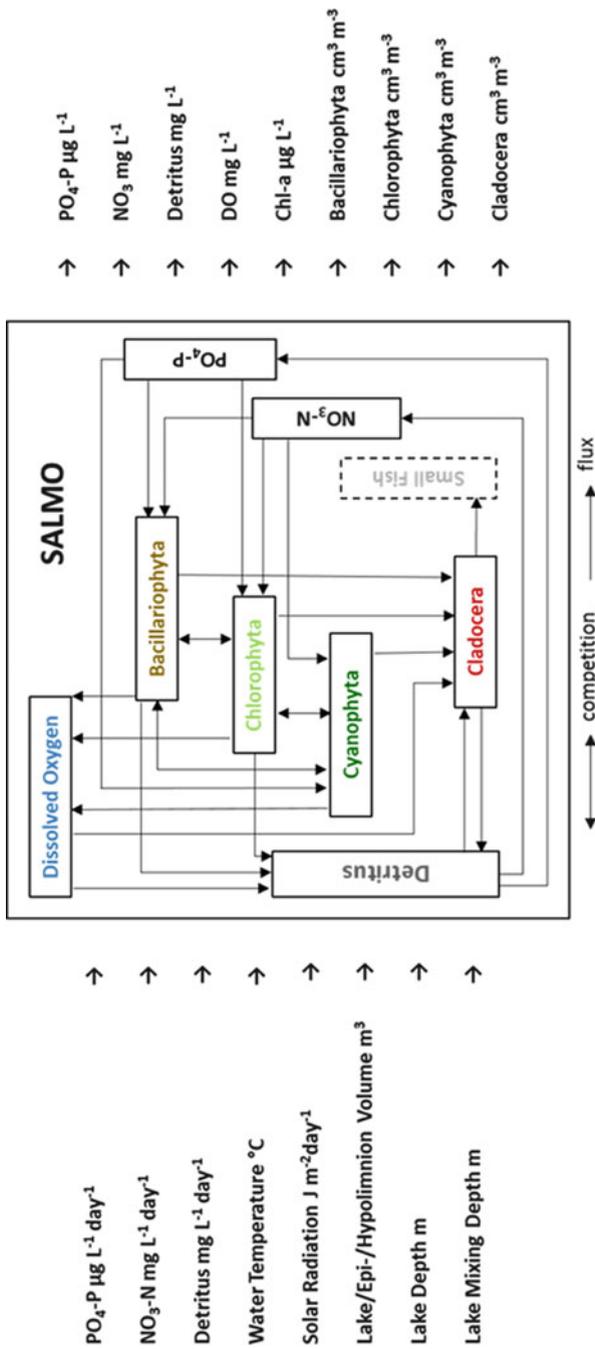


Fig. 10.3 Basic drivers, state variables and process pathways of the lake model SALMO

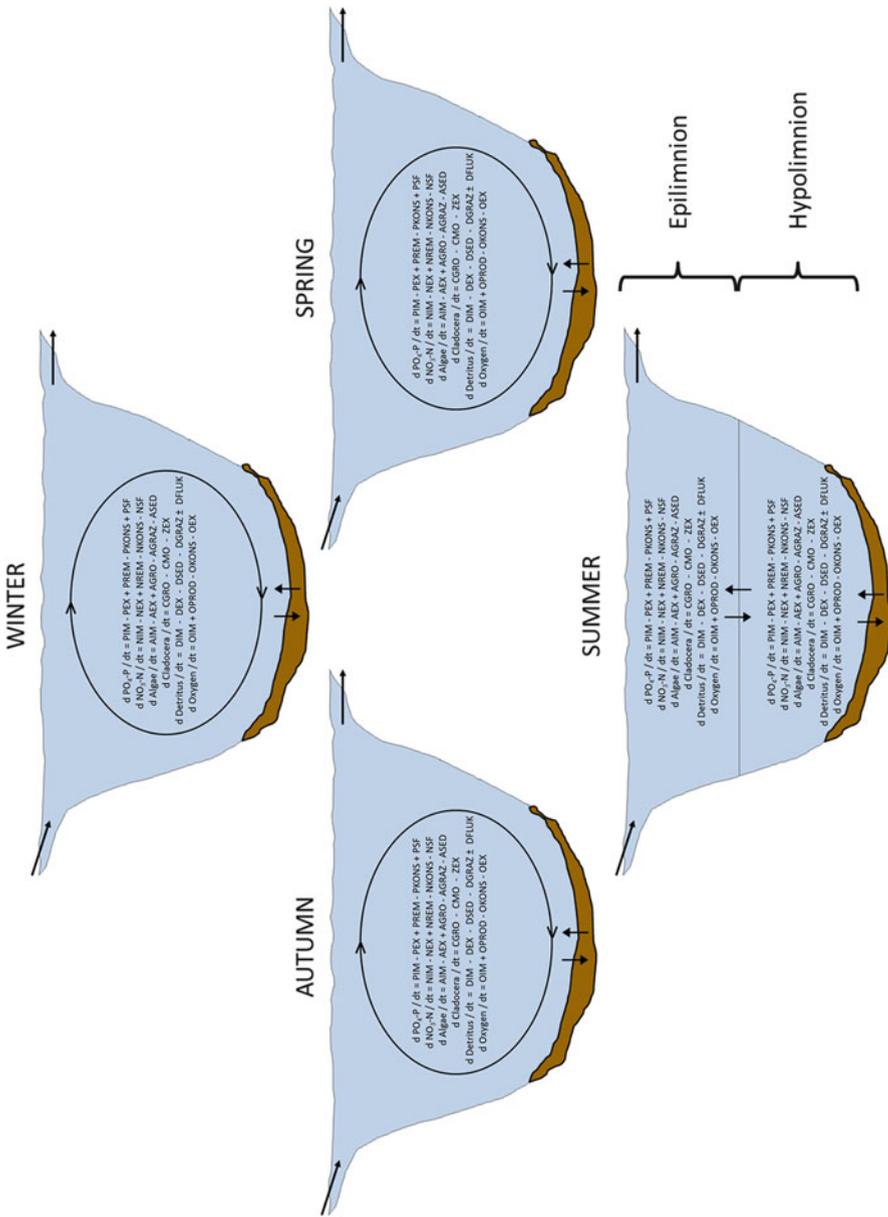


Fig. 10.4 Conceptual scheme for SALMO simulations of warm-monomictic lakes by seasonally alternating between a zero- and a one-dimensional model

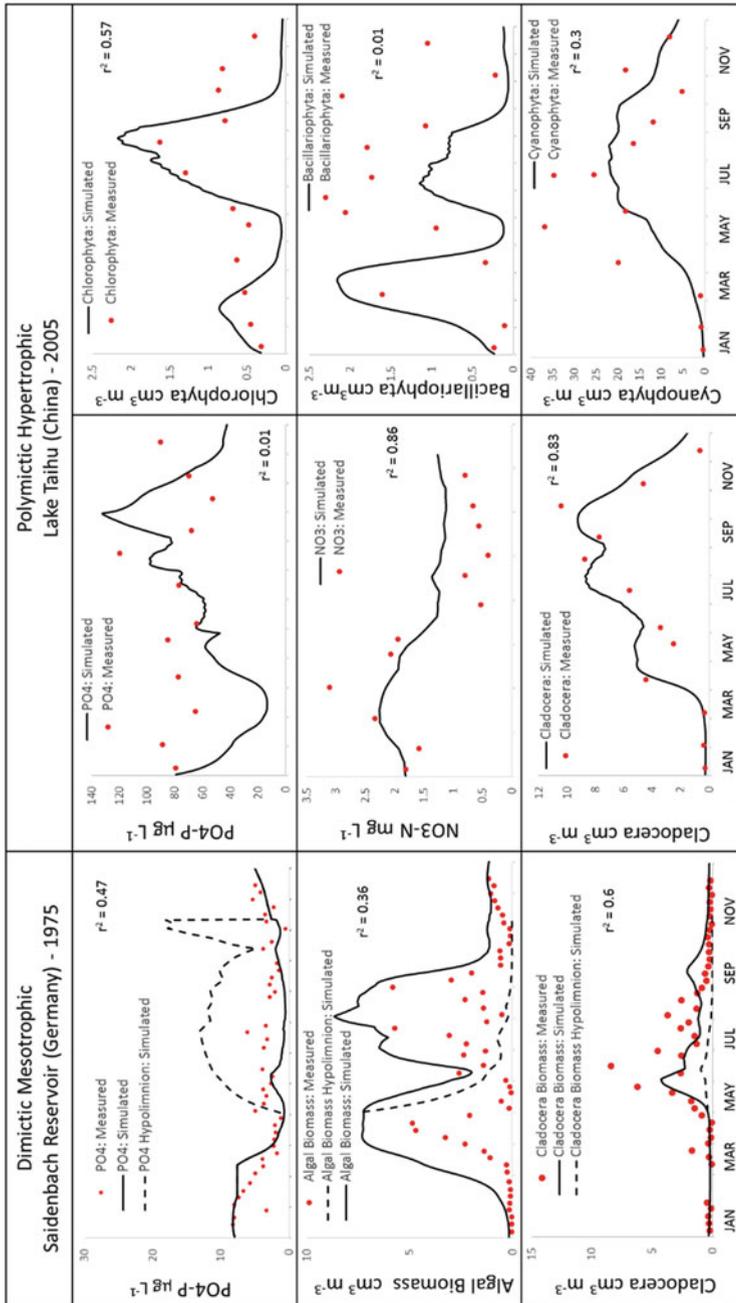


Fig. 10.5 Validation of SALMO for the dimictic mesotrophic Saldenbach Reservoir (*left column*) and the polymictic hypertrophic Lake Taihu (*middle and right columns*)

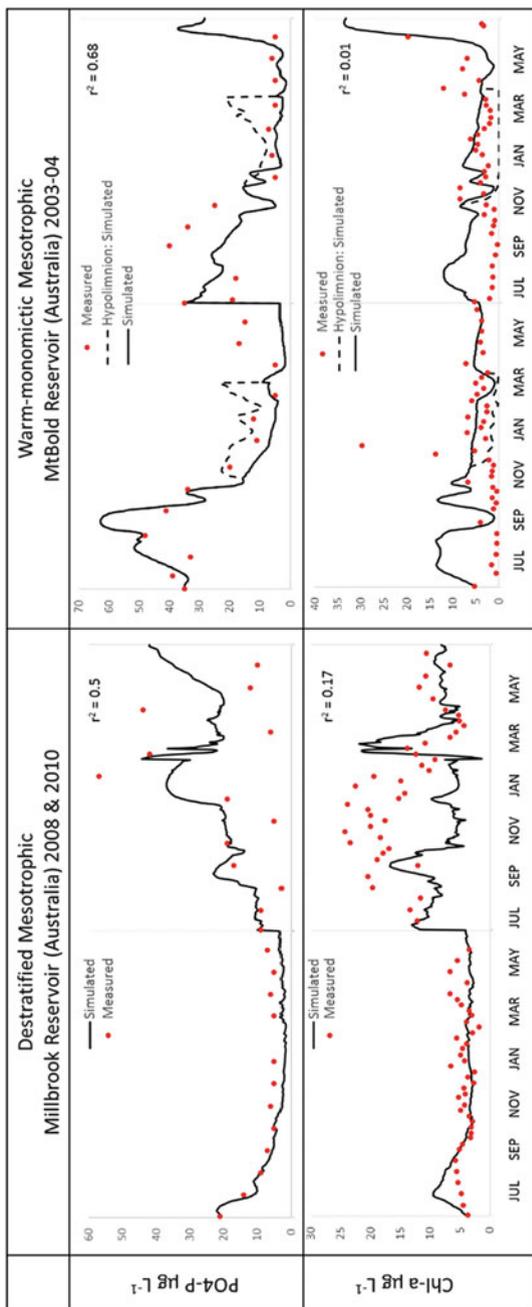


Fig. 10.6 Validation of SALMO for the destratified mesotrophic Millbrook Reservoir from 07/2008 to 06/2009 and 07/2010 to 06/2011 (*left column*) and the warm-monomictic mesotrophic Mt Bold Reservoir from 07/2003 to 06/2005 (*right column*)

ensemble SWAT-SALMO is applied to the Millbrook catchment-reservoir system. The Mt Bold Reservoir is thermally stratified during summer.

The performance of SALMO for different water bodies depends firstly on having accurate data for the key driving variables reflecting depths and volume fluctuations, nutrient loadings, light and temperature dynamics, secondly on having accurate measurements of key state variables for validation, and thirdly on correct calibration of phyto- and zooplankton related growth parameters reflecting nutrient, food, light and temperature limitations. The calibration of SALMO for specific water bodies focuses on key parameters determined by sensitivity analysis (e.g. Recknagel 1984) and their multi-objective optimization by evolutionary algorithms (Cao et al. 2008; Cao and Recknagel 2009; Chen et al. 2014) within the range of their standard error and against measured state variables.

10.3 Multi-dimensional Lake Models

The transition from 0-dimensional to higher dimensional models makes it necessary to include processes related to internal lake dynamics as well as more complex boundary conditions. Biogeochemical processes essentially stay the same, but we have to add different transport mechanisms driven by external and internal forces. While in the previous chapters, we focussed on the biogeochemical processes, here we examine physical processes changing the natural environment of a lake.

In a natural lake environment processes will be affected by driving forces at the surface—and to a lesser extend at the bottom—which may vary in time and space generating complex flow patterns in a lake. Driving forces such as weather or inflow will change the balance of heat and momentum in a lake, which can be described as an analogue to the previously mentioned mass balance. Physically speaking, to solve for processes in a real lake environment, we need to solve additional differential equations for velocity (momentum balance) at each point in the domain as well as for temperature (heat balance) or salinity (constituent mass balance), see e.g., Hutter and Jöhnk (2004). The resulting system of equations, Navier-Stokes equation and heat balance using Fourier's Law of heat conduction, is usually too complex to be solved directly and has to be adapted for specific situations. Knowing transport properties, advective and diffusive, throughout the lake then allows for the simulation of spread and distribution of constituents like nutrients, particulate matter or algae.

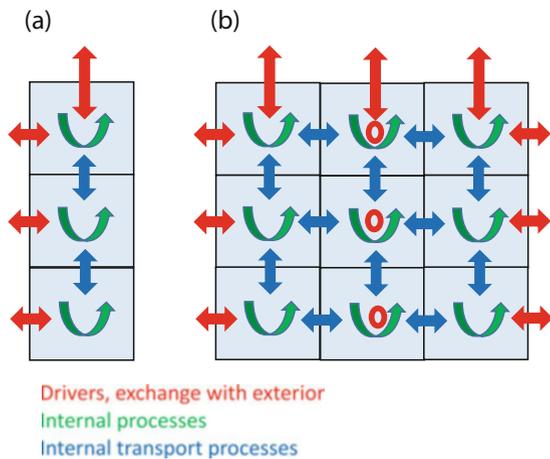
One simplification step is the separation of large from small-scale processes. This then leads to simplified equations describing the general flow or transport in a lake and a parameterization of small-scale process describing turbulence, i.e. diffusional transport. The latter can either be a set of extra differential equation like the k- ϵ turbulence model (e.g. Joehnke and Umlauf 2001), or a simplified version describing diffusional processes via a functional dependence on the vertical density gradient in a lake (or in physical terms better expressed as the buoyancy frequency). Another simplification, which can be well observed in oceans and

lakes, comes from the fact that these systems are to a large extent laterally homogeneous, i.e., in a lake changes mainly happen in the vertical as long as one is far away from a boundary. However, the smaller the system is, the more influence from the boundary needs to be taken into account, and the larger a lake or the more complex its bathymetry is the more likely three-dimensional flows will form.

In the previous examples of 1D lake models, it was assumed that lake stratification could be described by a two-layered system. This is a valid assumption, as long as the dynamic changes during build-up or breakdown of stratification are of no interest. Specific processes at the interface between these two layers are also neglected by such a simplifying assumption, e.g., a metalimnetic oxygen minimum (Joehnk and Umlauf 2001) where the system is determined by enhanced microbiological decomposition through accumulation in the metalimnion due to an increase in density.

In Fig. 10.7, different strategies for describing the spatial variability of a lake are depicted. In each compartment of such geometry, nutrient cycling and food web processes can be described individually. However, the more spatial complexity one needs to take into account, the more physical, transport processes have to be accounted for. In a zero dimensional system (Fig. 10.1a), e.g., a shallow well-mixed pond, no specific physical processes have to be looked at as long as the time scales of biogeochemical processes are larger than the time scales of turbulent processes mixing the system. A one-dimensional horizontal system (Fig. 10.1b), e.g. a channel type lake, might have well mixed conditions along its axis, horizontal transport processes have to be taken into account for this case. A classical example is the longitudinal decrease of dissolved oxygen in a river by degradation of biochemical oxygen demand (BOD) described by the Streeter-Phelps equation accounting for horizontal flow (Streeter and Phelps 1925). The one-dimensional vertical case (Fig. 10.1b) is an adequate description of a lake when neglecting horizontal gradients generated by boundary effects. Here, changes in the vertical

Fig. 10.7 Different process types in a one- (a) and a two-dimensional (b) discretization of a lake



are generated by turbulent and convective mixing, which are attributed to wind stress at its surface or heat loss from the surface. This is a widely used approach in describing lake dynamics. Numerous models exist to describe the hydrodynamics and thermal characteristics of this type of lake approximation (e.g. Stepanenko et al. 2013, 2014) including complex biogeochemical processes (see Janssen et al. 2015 for an overview).

The more small scale processes of a water body need to be included, the more knowledge on interacting bio-physical processes as well as on its geometry is required. For a 1-dimensional case it is assumed that the water body can be idealized by a set of serially connected “grid cells” (Fig. 10.7a). In a 2-dimensional case grids are connected across two dimensions—attaching a set of 1D cell structures (Fig. 10.7b), and finally a three-dimensionally resolved lake would consist of slices of 2-dimensional grids fitting the shape of lake morphometry and communicating across cell boundaries. While cell-internal biogeochemical processes are described as in the examples above, the exchange between cells and the prescription of driving forces at the cells’ external boundaries have to be defined based on physical principles (Fig. 10.7). This increase in geometric complexity also accompanies a higher complexity in physical processes (Wüest and Lorke 2003), which in most cases makes it necessary to significantly lower the time step (down to minutes or even seconds) of numerical solvers to resolve the various time scales of physical processes. For 1- and 2-dimensional systems, the computational overhead of running hydrodynamic and food web models in parallel is not restricted by current computing technology. However, for large 3D models (or for lower dimensional models running a multitude of scenarios) it may be necessary to decouple hydrodynamics from biological dynamics and using averaged (e.g. hourly or daily) physical quantities for the biological model parts (e.g. Skerratt et al. 2013). The necessary higher time resolution and spatial knowledge of drivers and boundary conditions for 2D- or 3D- is often not met with actual lake monitoring, in which case a reduction of geometric complexity is more adequate to describe the problem.

Large lakes and estuaries often have a very complex shape, which introduces a further complication in higher dimensional modelling of such systems. To adequately describe the geometry of e.g. small bays or river channels attached to the larger water body, it is necessary to either substantially reduce the grid spacing in these sub-systems, which would increase the CPU time, or to implement sub-gridding. The latter uses a higher resolved grid only for the specific region and communicates with the low-resolution grid via boundary conditions at its matching side, i.e., prescribed fluxes, water level, etc. This allows for fast calculation of the large-scale transport mechanisms and high resolution in the sub-grid region. In the Fitzroy Estuary attached to the Great Barrier Reef, Australia, such sub-gridding is used to simulate the spread of freshwater plumes from rivers during flood events. While the large scale grid size in this coastal system is of the order of 4 km, the sub-gridded region has resolutions down to 200 m. Figure 10.8 shows a snapshot of the salinity distribution in the estuary for the sub-gridded region in comparison to the large scale grid solution (red lines).

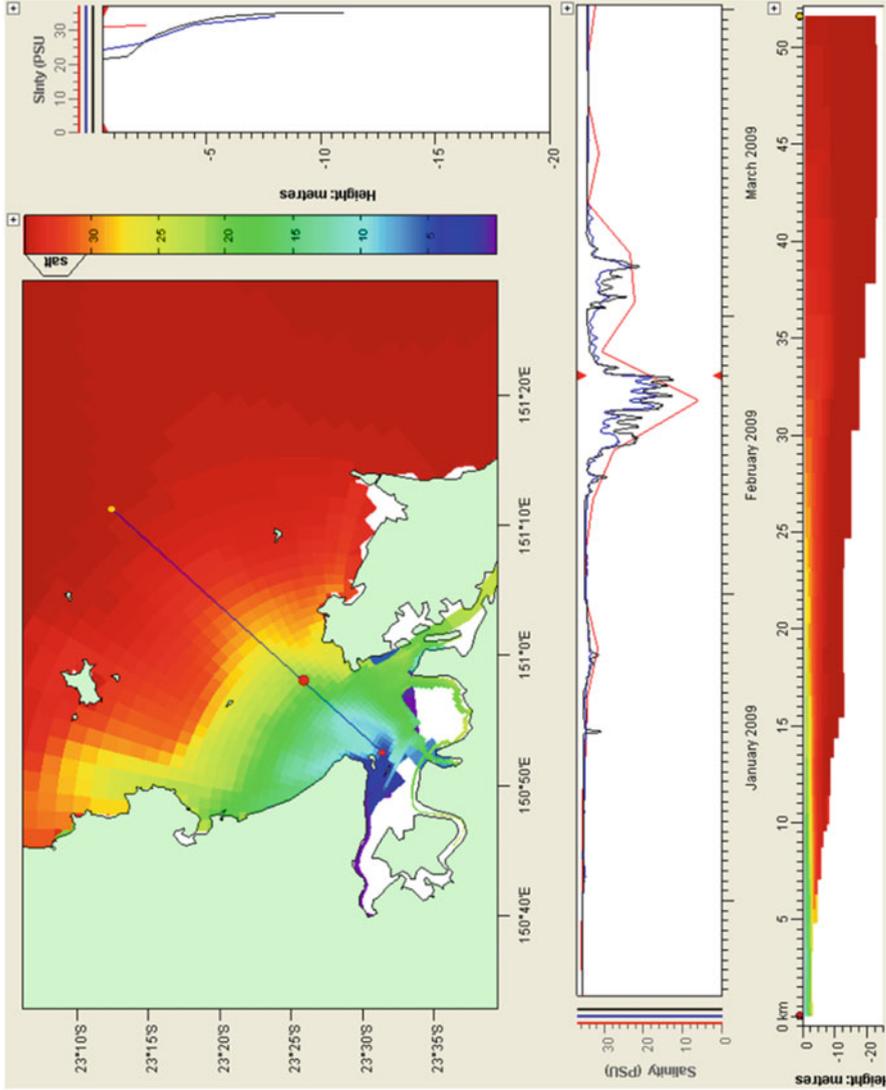


Fig. 10.8 Salinity simulation of river inflow into the Fitzroy Estuary, Australia, for a subgridded region (blue/black lines) in comparison to results for a large-scale ocean model (red lines). Profiles and time series are for the location in the middle of the estuary (red dot)

10.3.1 Horizontal and Vertical Transport of Nutrients and Organisms

Using simple connected regions for a lake, like the partitioning into epilimnion/hypolimnion for a food web model does not allow for a description of transport. Instead an exchange rate between compartments has to be described. This can be achieved by balancing the amount of constituents in the compartments over time and deriving the relative quantity of a constituent transferring over a time period from one into the adjacent compartment, e.g., particles sinking out of the epilimnion. For higher dimensional lake models with better spatial resolution, this process will be substituted with one based on physical transport mechanisms, i.e. advective transport of a quantity—temperature, particles, etc.—with a local velocity and re-distribution due to turbulent diffusion. The advective transport or velocity is a direct result of solving the hydrodynamic equations of motion in a lake. They describe a general flow pattern usually driven by wind action or inflow. Turbulent diffusion summarizes the small-scale processes generated by shearing in a fluid and due to local density instabilities. The latter is usually described as thermal instabilities when looking at freshwater systems, which are generated by surface cooling through heat loss usually during night-time. While the flow patterns act on time scales of hours to days or longer, the diffusional process describe fast processes with time scales of minutes or smaller. These diffusional processes are the drivers of constituent re-distribution in the water column. As such, the strength of turbulent diffusion will determine the amount of light a phytoplankton will be able to harvest while it is stochastically moved through the water column. Describing this motion through “diffusion” is again an approximation of the true process; it describes the mean distribution of a large amount of particles, but is not capable to follow the path of a single particle.

10.3.2 Multi-segment Lake Model for Studying Dreissenids and Macrophytes

The invasion of dreissenid mussels has been responsible for a major restructuring of the biophysical environment in many parts of the Laurentian Great Lakes, with profound alterations on the nutrient dynamics in the littoral zone (Coleman and Williams 2002). The nearshore shunt (sensu Hecky et al. 2004) has been hypothesized to impact the fate and transport of particulate matter, and subsequently alter the relative productivity of inshore sites and their interactions with the offshore areas. An important implication of the causal linkage between dreissenids and nutrient variability in the littoral zone is the weakening of the external loading signal, which led Hecky et al. (2004) to question whether conventional TP mass-balance models developed during the pre-dreissenid period in the Great Lakes were structurally adequate during the post-dreissenid era. In this context, Gudimov et al.

(2015) presented a mechanistic model designed to examine the role of macrophyte dynamics, to explicitly represent the impact of dreissenids in lakes, and to sensibly portray the interplay between water column and sediments.

In Lake Simcoe, Ontario, Canada, dreissenid mussel distribution is determined by a complex interplay among lake depth, substrate availability and exposure to wave disturbance (Ozersky et al. 2011; Evans et al. 2011). Specifically, the highest dreissenid biomass is typically found at areas of intermediate depth, where water movement is high enough to ensure that the lake bottom is dominated by rocky substrate but not excessively high to cause catastrophic disturbances to the dreissenid community. Gudimov et al. (2015) used their phosphorus mass-balance model to test the hypothesis that the spatial and temporal variability of P in Lake Simcoe was predominantly driven by internal mechanisms following the establishment of dreissenids. Because of the large size and complex shape of Lake Simcoe, a zero-dimensional spatial configuration would have been inadequate as the fundamental assumption that the lake is thoroughly mixed with uniform concentrations throughout is profoundly violated. On the other hand, there was not sufficient information (water levels, circulation patterns) to support the implementation of an explicit 2D or 3D hydrodynamic model. As an optimal compromise between the two strategies, the horizontal variability of Lake Simcoe was accommodated with four completely-mixed compartments, while the stratification patterns typically shaping the water quality in Kempenfelt Bay, Cook's Bay and the main basin were reproduced by the addition of three hypolimnetic compartments (Fig. 10.9, left panel). According to the Gudimov et al. (2015) model, the Lake Simcoe segmentation resembles Nicholls' (1997) conceptualization, in that the two embayments (Kempenfelt Bay and Cook's Bay) along with the shallow littoral zone at the east end (East Basin) are separated from the main basin (Fig. 10.9, left panel). The epilimnetic segments were interconnected through bi-directional hydraulic exchanges to account for wind-driven flows and tributary discharges from adjacent watersheds.

The Lake Simcoe model was designed to improve the fidelity of epilimnetic TP simulations through detailed specification of internal P recycling pathways (Fig. 10.9, left panel), such as the macrophyte dynamics and dreissenid activity as well as the fate and transport of P in the sediments, including the sediment resuspension, sorption/desorption in the sediment particles, and organic matter decomposition. Thus, the ordinary differential equations describing the dynamics of P in the water column consider all the external inputs, advective horizontal mass exchanges between adjacent segments, macrophyte uptake, macrophyte P release through respiration, dreissenid filtration, dreissenid excretion and pseudofeces egestion, vertical diffusive exchanges when stratification is established, and refluxes from the bottom sediments.

After the model calibration against the observed patterns in Lake Simcoe during the 1999–2007 period, Gudimov et al. (2015) first attempted to shed light on the role of the phosphorus fluxes associated with the dreissenid mussels. It was predicted that dreissenids filter a considerable amount of particulate P from the water column ($6.2\text{--}238$ tonnes P year⁻¹), but the effective clearance rate is

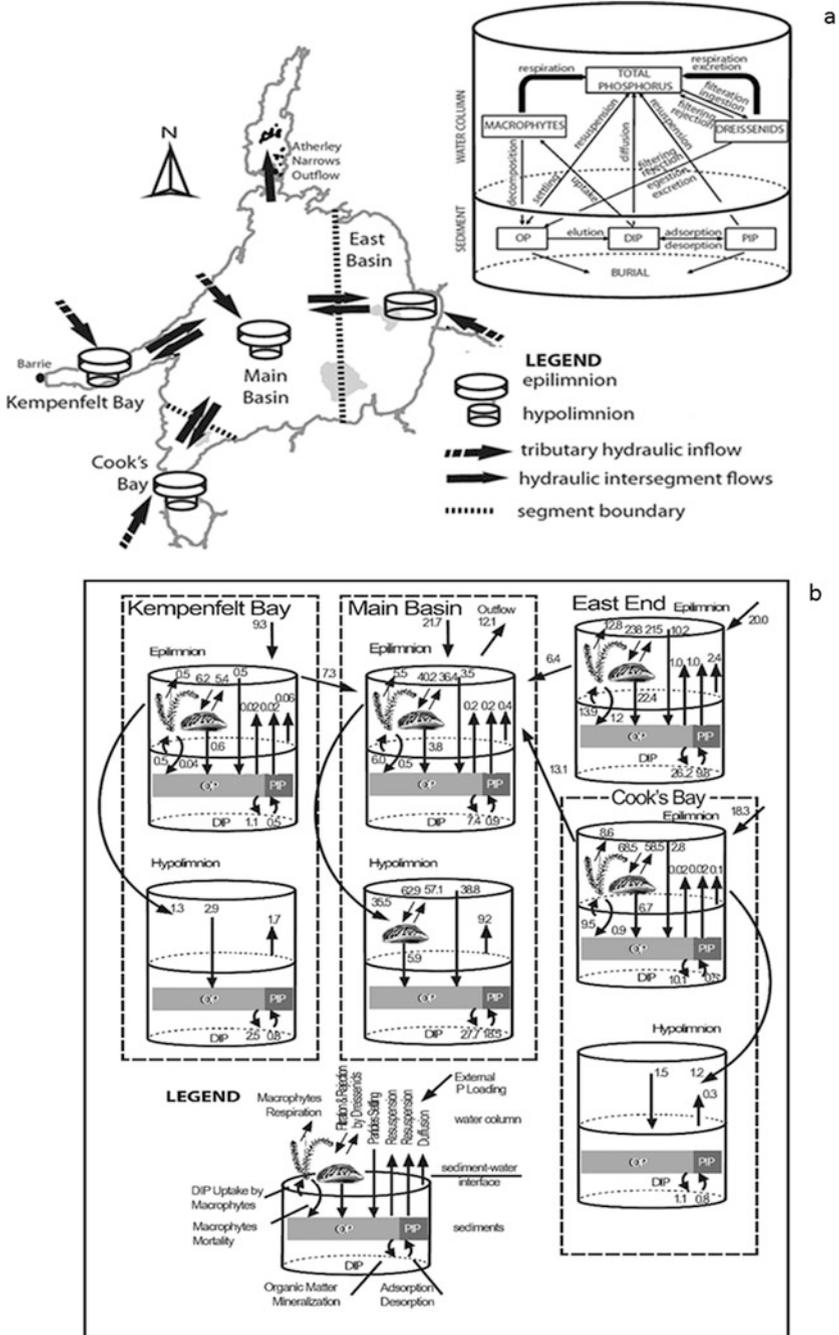


Fig. 10.9 Spatial segmentation and conceptual diagram of phosphorus pathways in the process-based model of Lake Simcoe (a). Simulated phosphorus fluxes (tonnes P year⁻¹) in water column and sediment layer in the spatial segments of Lake Simcoe (b)

significantly lower (0.8–22.8 tonnes P year⁻¹) with a substantial amount of the filtered particles (>85%) returned into the water column as feces, pseudofeces or other metabolic excreta. The latter finding is not surprising as the ratio between zebra mussel filtration and effective clearance rate can vary between 3.4 and 6.9 (Yu and Culver 1999). In particular, the Gudimov et al. (2015) study highlighted the critical role of dreissenids in the shallow eastern end of Lake Simcoe, where they filter 238.5 tonnes P year⁻¹ from the water column and subsequently egest 215.0 tonnes P year⁻¹, while an additional 22.4 tonnes P year⁻¹ of metabolic excreta are deposited onto the sediments. Because of its shallow morphometry, a large portion of the eastern area is located within the euphotic and well-mixed zone, and therefore the elevated benthic photosynthesis and access of the dreissenids to sestonic algae create favourable conditions for biodeposition and nutrient recycling (Ozersky et al. 2013). Importantly, the large fetch of Lake Simcoe, the relatively deep epilimnion, and the fairly rapid horizontal mixing often induce hydrodynamic conditions that may allow the localized impacts of dreissenids to shape ecosystem-scale patterns (Schwalb et al. 2013).

Consistent with empirical evidence from the system, the Lake Simcoe model predicted that macrophyte intake was responsible for a significant loss of P from the interstitial waters, thereby providing a significant pathway for the rapid transport of the nutrients assimilated from the sediments into the water column. P diffusive fluxes from the sediments accounted for about 30–35% of the exogenous P loading in Lake Simcoe. The retention capacity in Cook's Bay was estimated to be about 28%, which is distinctly lower than estimates from the 1980s. Thus, the colonization of the embayment by dreissenids and the recent proliferation of macrophytes appear to have decreased the P retention in Cook's Bay, where the predominant fraction of TP is carbonate-bound P (apatite-P) mainly due to the accelerated erosion in the catchment (Dittrich et al. 2012). The sediments in the main basin are mostly driven by fast diagenetic processes of settling organic matter from the epilimnion, resulting in internal P loading of 9.2 tonnes P year⁻¹. In a similar manner, the hypolimnetic sediments in Kempenfelt Bay are responsible for a fairly high diffusive P flux into the water column (≈ 1.7 tonnes P year⁻¹), presumably reflecting the highest proportion of the redox-sensitive P sediment pool compared to other lake segments (Dittrich et al. 2012).

10.4 Concluding Remarks

As knowledge regarding the complex components of environmental systems continues to grow, there is a demand for increasing the articulation level of our mathematical models. Generally, the premise for constructing complex models is to mirror the complexity of natural systems and consider ecological processes that can become important in future states and are driven by significantly different conditions. Modelers essentially believe in the myth that if they can include 'all' the significant processes in the mathematical equations, then the model will closely

mimic the 'real system' and thus will have increased predictive ability under a wide range of environmental conditions. However, there is always a trade-off between model complexity, transparency, uncertainty and validity, as well as data obtainability. Increasing computational potential is tempting to solve biogeochemical models in a 2- or 3-dimensional manner to cope with lateral changes in aquatic systems as well as including more complex physical transport phenomena (MacKay et al. 2009). However, this requires an adequate level of in-lake monitoring but also access to large scale resolved meteorological data as drivers of physical processes. Assimilation of remote sensing data with hydrodynamic modelling (e.g. Pinardi et al. 2015) may further improve predictive abilities of models (see also Chap. 15).

In the context of aquatic biogeochemical modeling, there is increasing pressure to explicitly treat multiple biogeochemical cycles, to increase the functional diversity of biotic communities, and to refine the mathematical description of the higher trophic levels (Arhonditsis and Brett 2004; Anderson 2005; Fennel 2008). In particular, there are views in the literature suggesting the inclusion of multiple nutrients along with the finer representation of plankton communities, as necessary model augmentations for disentangling critical aspects of aquatic ecosystem dynamics, e.g., species populations are more sensitive to external perturbations (nutrient enrichment, episodic meteorological events), and key biogeochemical processes are tightly linked to specific plankton functional groups (Flynn 2005). Nonetheless, the derivation of distinct functional groups from fairly heterogeneous planktonic assemblages poses challenging problems. Because of the still poorly understood ecology, we do not have robust group-specific parameterizations that can support predictions in a wide array of spatiotemporal domains (Anderson 2005).

Preliminary efforts to incorporate plankton functional types into global biogeochemical models were based on speculative parameterization and, not surprisingly, resulted in unreliable predictions (Anderson 2005). In the same context, a recent meta-analysis evaluated the ability of 124 aquatic biogeochemical models to reproduce the dynamics of phytoplankton functional groups (Shimoda and Arhonditsis 2016). Most notably, moderate fit statistics were found for diatoms (median $r^2 = 0.31$, RE = 70%) and cyanobacteria (median $r^2 = 0.36$, RE = 65%), and even worse performance was recorded for cryptophytes (median $r^2 = 0.39$, RE = 79%), flagellates (median $r^2 = 0.07$, RE = 78%) and haptophytes (median $r^2 = 0.39$, RE = 41%), which likely reflects our limited knowledge of their ecophysiological parameters compared to other well-studied functional groups. Significant variability also exists with respect to the mathematical representation of key physiological processes (e.g. growth strategies, nutrient kinetics, settling velocities) as well as group-specific characterizations typically considered in the pertinent literature. Furthermore, recent attempts to integrate biogeochemistry with fish production underscore the uncertainty arising from the mismatch between the operating time scales of planktonic processes and fish life cycles as well as the need to consolidate the mechanistic description and parameterization of several critical processes, such as the reproduction and mortality of the adult stages (Fennel 2008). Despite repeated efforts to increase model complexity, we still have not gone

beyond the phase of identifying the unforeseeable ramifications and the challenges that we need to confront so as to improve the predictive power of our models. Until we have the knowledge to mathematically depict the interplay among physical, chemical, and biological processes with greater fidelity and less uncertainty, the gradual incorporation of model complexity, where possible and relevant, is the most prudent strategy. The Bayesian analysis of model uncertainty will be addressed in detail in Chap. 11.

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